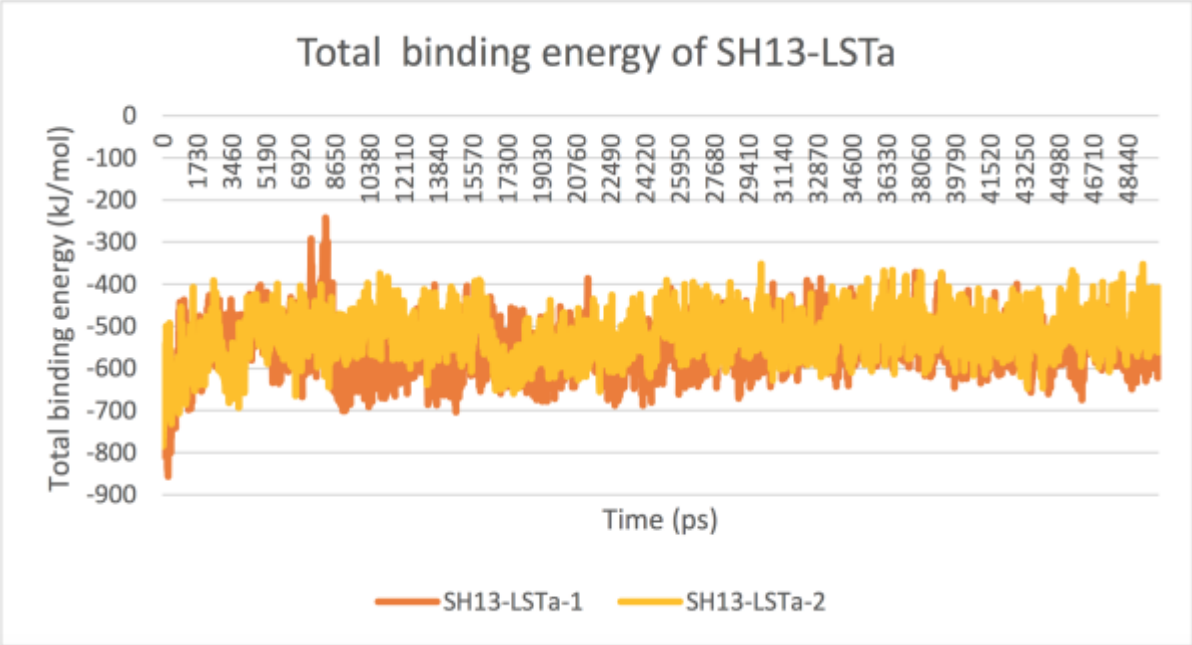
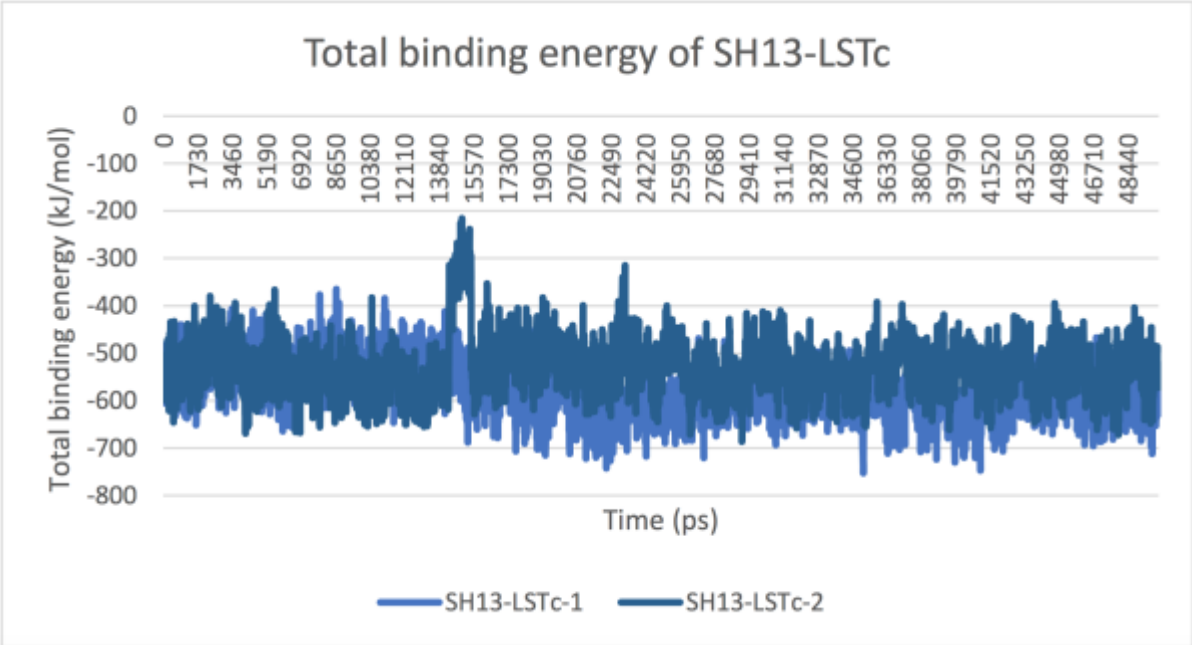
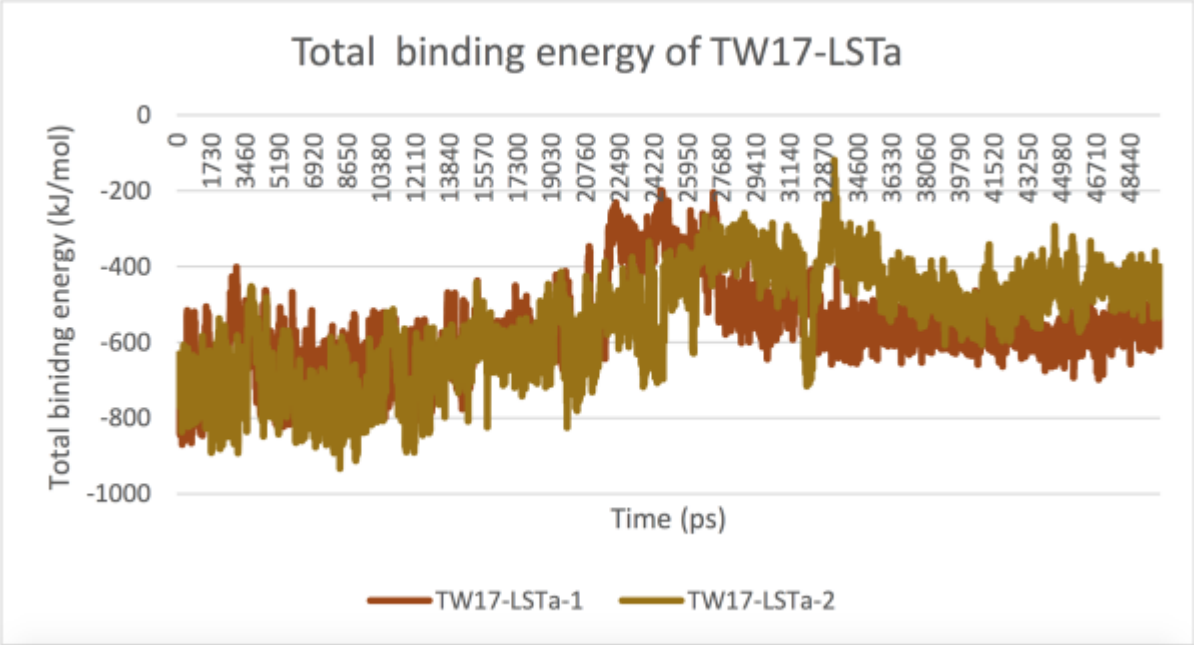
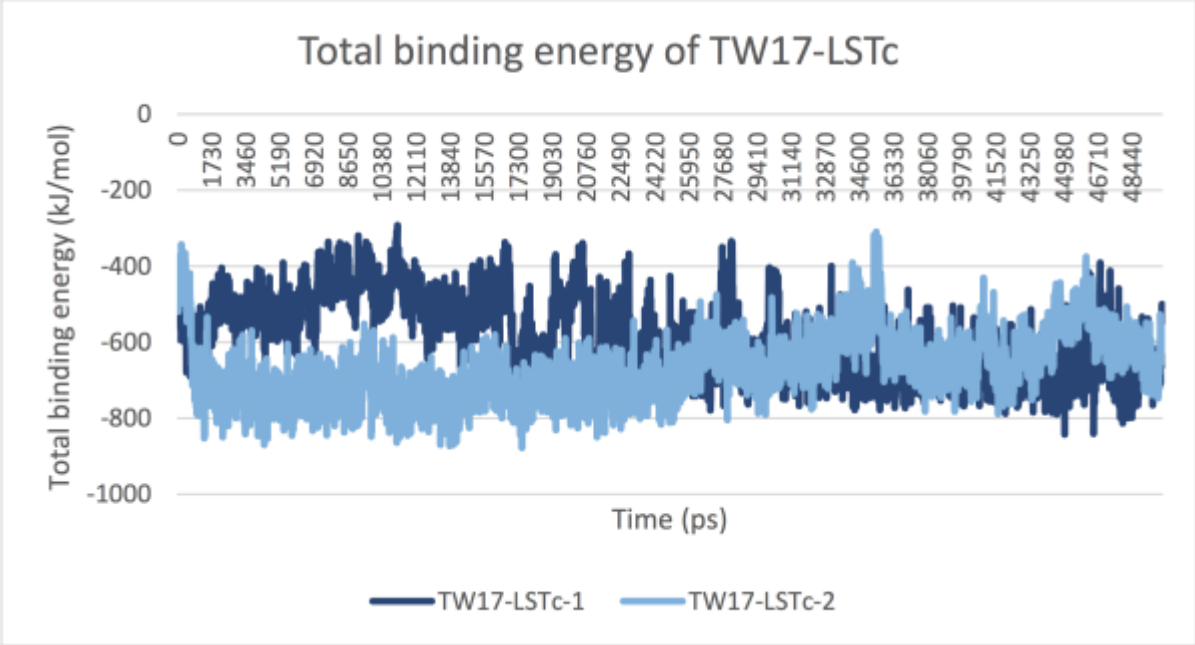
Additional file 4. Two rounds of 50 ns molecular dynamics simulation for SH13-LSTa, SH13-LSTc, TW17-LSTa, TW17-LSTc

we conducted two rounds 50 ns molecular dynamics simulation. The total binding energy for each system has been shown in the following figures.









The averages of total binding energy for the HA-LSTa/LSTc complexes are listed in Table 1. The results are consistent with the main text. The mutant TW17 HA obtains the largest binding energy, and enhances the binding with two types receptors, especially LSTc. Both SH13 and TW17 strains have binding preference to LSTc. Additional file 6 shows the simulation results of each system and the average total binding energy.

Table 1. Average total binding energy (kJ/mol) of the HA-LSTa/LSTc complexes.

	LSTa	**LSTc**	**$^{1}\Delta E_1$**
SH13	-539.168	-554.499	+15.331
TW17	-557.506	-633.218	+75.712
$^{2}\Delta E_2$	+18.338	+78.719	

1 Binding preference of HA protein: $\Delta E_1 = \Delta E_{HA,\ LSTa} - \Delta E_{HA,\ LSTc}$

2 Difference of HAs binding to receptors: $\Delta E_2 = \Delta E_{SH13,\ receptor} - \Delta E_{TW17,\ receptor}$